

3«beta»-Hydroxystigmast-5-en-7-one

Inchi: InChI=1S/C29H48O2/c1-7-20(18(2)3)9-8-19(4)23-10-11-24-27-25(13-15-29(23,24)6)28(5)
InchiKey: ICFXJOAKQGDRCT-CGUUZUFZSA-N
Formula: C29H48O2
SMILES: CCC(CCC(C)C1CCC2C3C(=O)C=C4CC(O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 428.69

Physical Properties

Property code	Value	Unit	Source
gf	95.29	kJ/mol	Joback Method
hf	-671.49	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	98.15	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.204		Crippen Method
mvol	379.170	ml/mol	McGowan Method
pc	980.23	kPa	Joback Method
rinpol	3609.00		NIST Webbook
rinpol	3609.00		NIST Webbook
tb	1060.52	K	Joback Method
tc	1299.59	K	Joback Method
tf	603.15	K	Joback Method
vc	1.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1515.22	J/mol×K	1060.52	Joback Method
cpg	1550.55	J/mol×K	1100.36	Joback Method
cpg	1587.08	J/mol×K	1140.21	Joback Method
cpg	1625.16	J/mol×K	1180.05	Joback Method
cpg	1665.18	J/mol×K	1219.90	Joback Method
cpg	1707.49	J/mol×K	1259.74	Joback Method
cpg	1752.46	J/mol×K	1299.59	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R641157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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